# 17<sup>th</sup> Electromagnetic and Light Scattering Conference College Station, TX, USA 4–9 March 2018

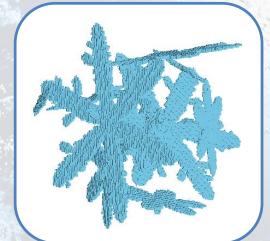


# Numerically Efficient Direct Solver-Based Full-Wave Model for EM Scattering from Complex-Geometry Particles

Ines Fenni\*, Ziad S. Haddad\*, Hélène Roussel\*\*, Raj Mittra#

\* Jet Propulsion Laboratory, California Institute of Technology, USA \*\* Sorbonne University, L2E-UR, France, # University of Central Florida, USA







### **Outline**



### 1) Motivations

- Increasing need for accurate and numerically efficient model of EM scattering from particles of arbitrary geometry and composition.
- Limitations of iterative solvers-based Discrete Dipole Approximation (DDA) codes

### 2) VIEM-MoM/CBFM

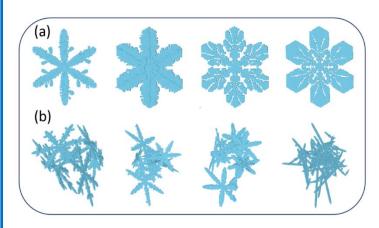
- VIEM/MoM-based 3D full wave model for scattering by complex-shaped precipitation particles.
- Application of the domain decomposition-based CBFM

### 3) Numerical Analysis

- Primary Validation of NESCoP by comparison to Mie theory
- Application of NESCoP vs DDSCat to different types of complex-geometry and electrically large particles



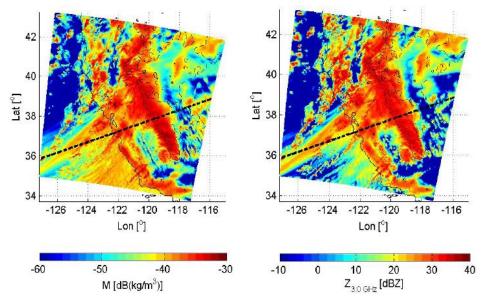
Z. S. Haddad & al, "Derived Observations From Frequently Sampled Microwave Measurements of Precipitation—Part I: Relations to Atmospheric Thermodynamics," in IEEE Transactions on Geoscience and Remote Sensing, June 2017.



Pristine crystals (a) & aggregate (b) snow particles from OpenSSP database



Single-scattering properties of particles with complex arbitrary geometries modeling ice pristine and snowflakes.



WRF simulations of the California blizzard: maps of condensed-water mass and S-band radar reflectivity

**Scattering Lookup Tables** 



$$Z(x,h) =$$

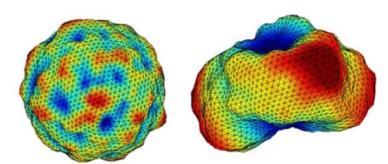
$$Z(x,h) = \sum_{i=1}^{N_{\text{species}}} Z_{u,i}(x,h) \times \exp \left[-2 \int_{h}^{\infty} X_{u,i}(x,h) \right]$$

$$-2\int_{h}^{\infty}\sum_{i=1}^{N_{\text{specie}}}$$

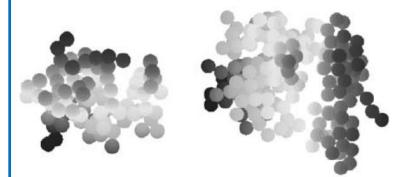
$$\sum_{i=1}^{\text{vspecies}} k_{\text{ext},j}(x,h') dh$$



Mollon, Guilhem, and Jidong Zhao. "3D generation of realistic granular samples based on random fields theory and Fourier shape descriptors." Computer Methods in Applied Mechanics and Engineering 2014.

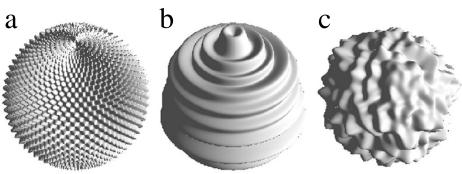


Mishchenko, Michael I., and Janna M. Dlugach. "Radar polarimetry of Saturn's rings: Modeling ring particles as fractal aggregates built of small ice monomers." Journal of Quantitative Spectroscopy and Radiative Transfer 2009



Single-scattering properties of particles with complex arbitrary geometries.

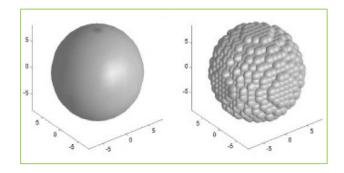
Different types of particles in nature: mineral aerosol particles in planetary atmospheres, cosmic dust particles, regolith particles on the surface of terrestrial planets and asteroids, ice-cloud particles...



## (a) 3D Chebyshev particles, (b) 2D and (c) 3D Gaussian random spheres

Kahnert, Michael, et al. "Light scattering by particles with small-scale surface roughness: comparison of four classes of model geometries." Journal of Quantitative Spectroscopy and Radiative Transfer, 2012.





Discrete dipole approximation (DDA) representation of a sphere



Single-scattering properties of particles with complex arbitrary geometries.



Discrete Dipole approximation

(DDA): DDScat, ADDA, SIRRI, ...



 $|\mathbf{m}|\mathbf{kd} = \mathbf{0.6}$ 

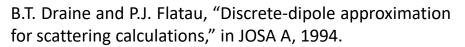


### Validity criteria : |m|kd ≤ 1

**m**: complex refractive index

k: wavelength number

d: grid spacing

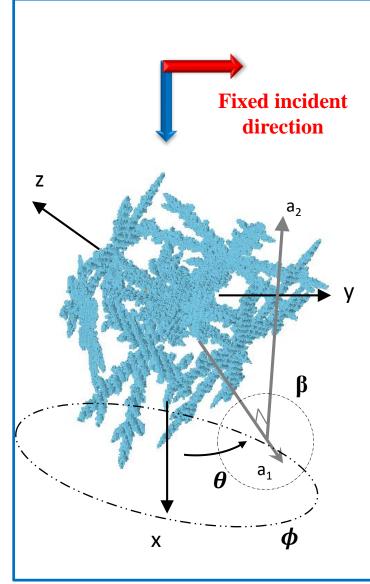


Penttilä, Antti, et al. "Comparison between discrete dipole implementations and exact techniques." *JQSRT*, 2007

Zubko, Evgenij, et al. "Validity criteria of the discrete dipole approximation." Applied optics, 2010









Single-scattering properties of particles with complex arbitrary geometries.



**Discrete Dipole approximation** 

(DDA): DDScat, ADDA, SIRRI, ...

**Iterative solvers**: Krylov-space methods, such as conjugate gradient (**CG**), Bi-CG, Bi-CG stabilized (**Bi-CGSTAB**), CG squared (**CGS**), generalized minimal residual (GMRES),

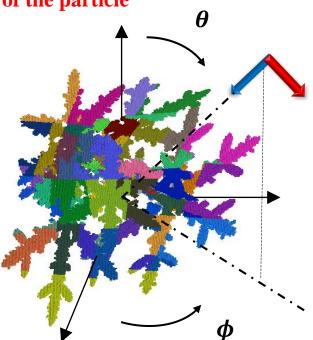
### **Orientation averaging**

$$\langle Q \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} d\beta \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi \ Q(\beta, \theta, \phi)$$

Yurkin, Maxim A., and Alfons G. Hoekstra. "The discrete dipole approximation: an overview and recent developments." Journal of Quantitative Spectroscopy and Radiative Transfer, 2007



# Fixed orientation of the particle



$$ZE = E^{inc}$$

**Direct solver** 



Single-scattering properties of electrically large and complex-geometry particles.



**Discrete Dipole approximation** (DDA): DDScat, ADDA, SIRRI, ...



Characteristic Basis Function Method (Domain decomposition method)

### **Orientation averaging**

$$\langle Q \rangle = \frac{1}{4\pi} \int_0^{2\pi} d\phi_i \int_0^{\pi} \sin\theta_i \ d\theta_i \ Q(\phi_i, \theta_i)$$

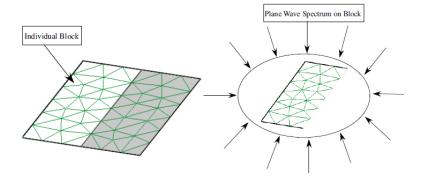
Singham, M. K., Shermila B. Singham, and Gary C. Salzman. "The scattering matrix for randomly oriented particles." *The Journal of chemical physics* 85.7 (1986)

### The Characteristic Basis Function Method (CBFM)



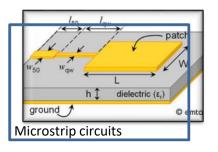
#### **Direct solver-based**

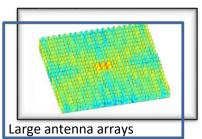
- ❖ Better adapted to multiple right-hand side problem
- Subject to a wide variety of enhancement techniques
- ❖ Tunable depending on to the needs (memory or CPU) through the size of the blocks (h<sub>B</sub> or N<sub>b.max</sub>).
- ❖ Highly amenable to MPI parallelization

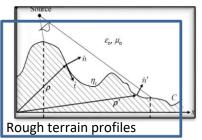


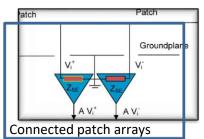
Spectrum of plane waves incident on a single block

The **CBFM** which has been proven to be accurate and efficient when applied to large-scale EM problems, even when the computational resources are limited



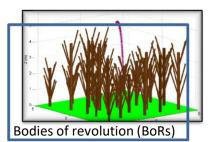






R. Maaskant, R. Mittra, A. Tijhuis, "Fast Analysis of Large Antenna Arrays Using the Characteristic Basis Function Method and the Adaptive Cross Approximation Algorithm", IEEE Transactions on Antennas and Propagation, 2008.

Jaime Laviada et al, "Solution of Electrically Large Problems With Multilevel Characteristic Basis Functions", IEEE Trans. on Antennas Propagation, 2009.



### **Outline**



### 2) VIEM-MoM/CBFM

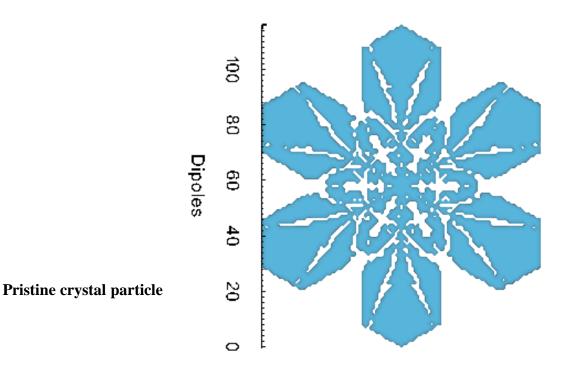
- VIEM/MoM-based 3D full wave model for scattering by complex-shaped precipitation particles.
- Application of the domain decomposition-based CBFM

### 3) Numerical Analysis

- Primary Validation of NESCoP by comparison to Mie theory
- Application of NESCoP vs DDSCat to different types of complex-geometry and electrically large particles



#### 3D full-wave model, based on the volume integral equation method (VIEM)



where  $\chi(r')$  is the dielectric contrast at the location r',  $k_0$ is the wavenumber in air and  $\overline{\overline{G}}$  ( $\overline{r}$ ,  $\overline{r}$ ') is the free space dyadic Green's function.



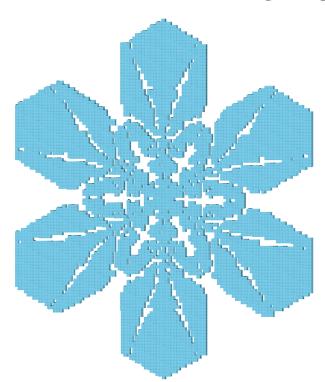
$$\overline{\bar{\Gamma}}\overline{E}(\bar{r}) = \overline{E}^{ref}(\bar{r})$$

$$\overline{\bar{\Gamma}}\overline{E}(\overline{r}) = \overline{E}^{ref}(\overline{r}) \qquad \text{where} \quad \overline{\bar{\Gamma}} = \overline{\bar{I}} - \left(k_0^2 + \nabla \nabla \cdot\right) \int_{\Omega} \chi(\overline{r}') \, \overline{\bar{G}}(\overline{r}, \overline{r}') \, d\overline{r}'$$



#### 3D full-wave model, based on the volume integral equation method (VIEM)

Pristine crystal particle discretized into Nb<sub>c</sub> elementary cubic cells



$$\overline{\overline{\Gamma}}\overline{E}(\overline{r}) = \overline{E}^{ref}(\overline{r})$$

#### **Method of Moments**

The particle is discretized into **Nbc** cubic cells  $\Omega_n$ , of side  $S_c$ 

$$S_c \leq \frac{\lambda_s}{10}$$
;  $\lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$ 

 $\mathbf{D}_{\lambda} = \lambda_{\mathrm{s}} / \mathbf{S}_{\mathrm{c}}$ 

$$\overline{E}(\overline{r}) = \sum_{n=1}^{N} \sum_{q=1}^{3} E_q^n \ \overline{F}_q^n(\overline{r})$$

Use of piecewise constant basis functions

Z is the 3Nb<sub>c</sub> x 3Nb<sub>c</sub> full matrix representing the interactions between the different cells.

 $ZE = E^{inc}$ 

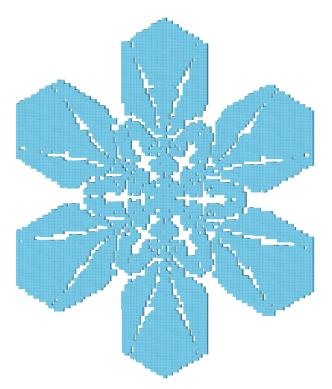


#### 3D full-wave model, based on the volume integral equation method (VIEM)

Pristine crystal particle discretized into Nb<sub>c</sub> elementary cubic cells



Z is the 3Nb<sub>c</sub> x 3Nb<sub>c</sub> full matrix representing the interactions between the different cells.



$$\overline{\overline{\Gamma}}\overline{E}(\overline{r}) = \overline{E}^{ref}(\overline{r})$$

#### **Method of Moments**

The particle is discretized into **Nbc** cubic cells  $\Omega_n$ , of side  $S_c$ 

$$|S_c| \leq \frac{\lambda_s}{10}$$
;  $\lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$ 

 $\mathbf{D}_{\lambda} = \lambda_{\mathrm{s}} / \mathbf{S}_{\mathrm{c}}$ 

$$\overline{E}(\overline{r}) = \sum_{n=1}^{N} \sum_{q=1}^{3} E_q^n \ \overline{F}_q^n(\overline{r})$$

Use of piecewise constant basis functions

 $ZE = E^{inc}$ 



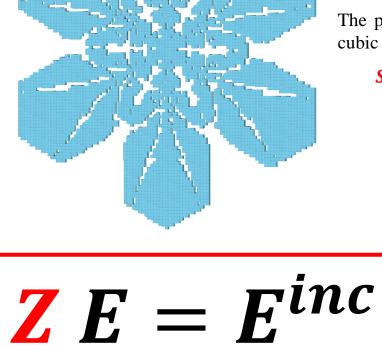
#### 3D full-wave model, based on the volume integral equation method (VIEM)

Pristine crystal particle discretized into Nb<sub>c</sub> elementary cubic cells



Z is the 3Nb<sub>e</sub> x 3Nb<sub>e</sub> full matrix representing the interactions between the different cells.

**CBFM** 



$$\overline{\overline{\Gamma}}\overline{E}(\overline{r}) = \overline{E}^{ref}(\overline{r})$$

#### **Method of Moments**

The particle is discretized into Nbc cubic cells  $\Omega_n$ , of side  $S_c$ 

$$S_c \leq \frac{\lambda_s}{10}$$
;  $\lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$ 

 $\mathbf{D}_{\lambda} = \lambda_{\mathbf{s}} / \mathbf{S}_{\mathbf{c}}$ 

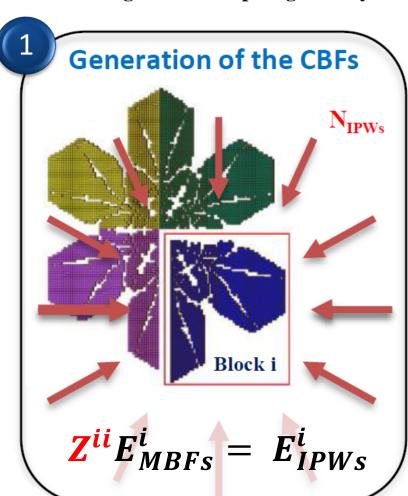
$$\overline{E}(\overline{r}) = \sum_{n=1}^{N} \sum_{q=1}^{3} E_q^n \ \overline{F}_q^n(\overline{r})$$

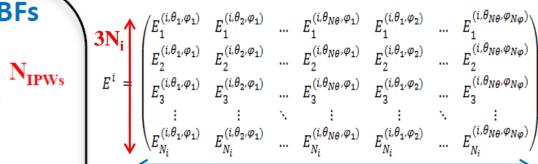
Use of piecewise constant basis **functions** 





#### After dividing the 3D complex geometry of the precipitation particle of N cells into M blocks





N<sub>IPWs</sub>

**Singular Value Decomposition (SVD)** 



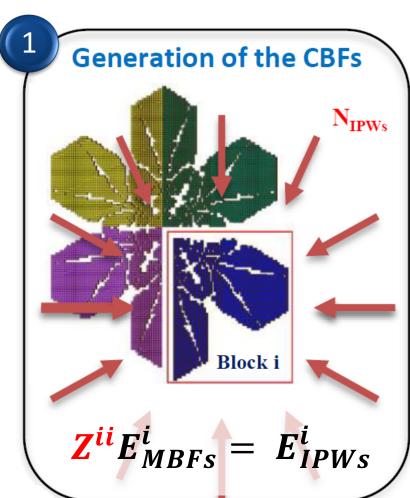
Normalization and thresholding (10<sup>-3</sup>)

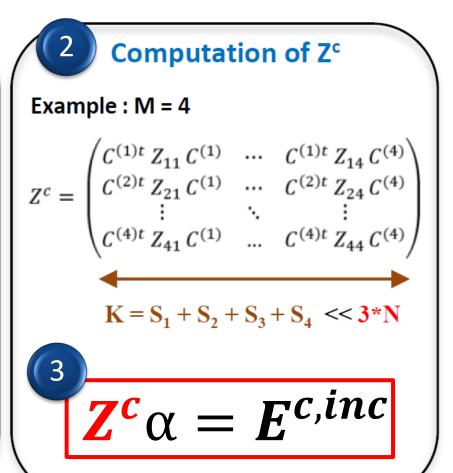


S<sub>i</sub> characteristic basis functions (CBFs) for the block i



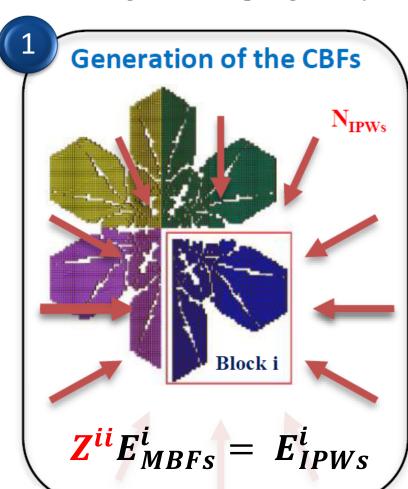
After dividing the 3D complex geometry of the precipitation particle of N cells into M blocks







After dividing the 3D complex geometry of the precipitation particle of N cells into M blocks



2 Computation of **Z**<sup>c</sup>

Example : M = 4

$$Z^{c} = \begin{pmatrix} C^{(1)t} Z_{11} C^{(1)} & \cdots & C^{(1)t} Z_{14} C^{(4)} \\ C^{(2)t} Z_{21} C^{(1)} & \cdots & C^{(2)t} Z_{24} C^{(4)} \\ \vdots & \ddots & \vdots \\ C^{(4)t} Z_{41} C^{(1)} & \cdots & C^{(4)t} Z_{44} C^{(4)} \end{pmatrix}$$

$$K = S_1 + S_2 + S_3 + S_4 << 3*N$$

**Compression Rate** 

$$CR = \frac{size \ of \ Z}{size \ of \ Z^c}$$







CBFM CBFs : O(3N/M)<sup>3</sup>

**Z**<sup>c</sup>: O(3N x K)

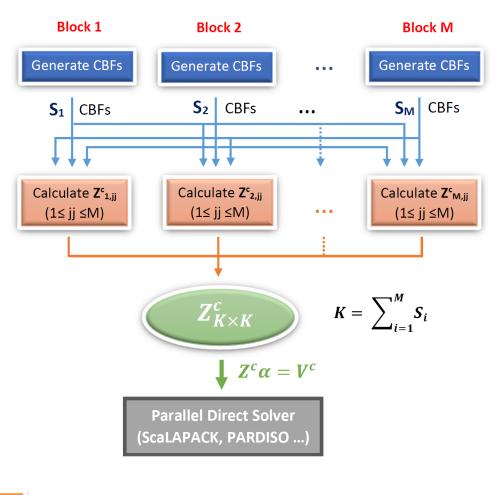
 $(Z^c)^{-1}:O(K)^3$ 



MPI

ACA/FMM

Efficient direct



The main steps of the CBFM in a distributed memory parallel configuration

### **Outline**



### 3) Numerical Analysis

- Primary Validation of **NESCoP** by comparison to **Mie theory**
- Application of NESCoP vs DDSCat to different types of complex-geometry and electrically large particles



### Orientational averaging

$$\langle Q \rangle = \frac{1}{4\pi} \int_0^{2\pi} d\phi_i \int_0^{\pi} \sin\theta_i \ d\theta_i \ Q(\phi_i, \theta_i)$$

Incident directions (id) –  $(\theta, \phi)$ 

$$Q\rangle = \frac{1}{8\pi^2} \int_0^{2\pi} d\boldsymbol{\beta} \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi \ Q(\boldsymbol{\beta}, \boldsymbol{\theta}, \boldsymbol{\phi})$$

 $\Rightarrow$  Target orientations (to) – ( $\theta$ ,  $\beta$ )

### Scattering Efficiency Coefficients

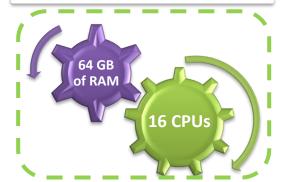
$$Q_{ext} = C_{ext} / \pi a^2$$

$$Q_{sca} = C_{sca} / \pi a^2$$

$$Q_{bks} = C_{bks} / \pi a^2$$

$$\begin{pmatrix} E_{\parallel \text{sca}} \\ E_{\perp \text{sca}} \end{pmatrix} = \frac{\exp(\mathrm{i}k_{\text{sca}}r)}{-\mathrm{i}k_{\text{sca}}r} \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} E_{\parallel \text{in}} \\ E_{\perp \text{in}} \end{pmatrix}$$

#### Shared Memory / OpenMP

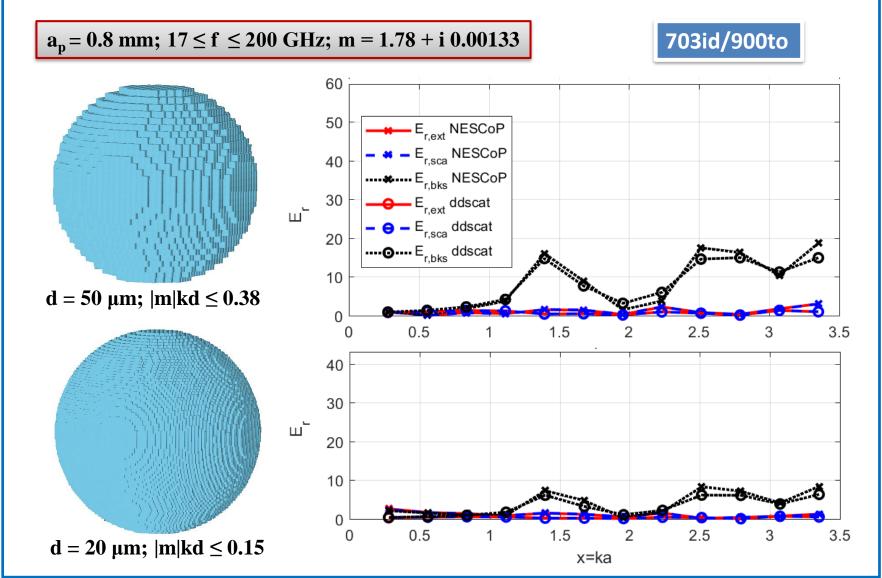


### Relative 'difference' (per frequency)

$$E_{r,t}(\%) = 100 \times \frac{|Q_{t,NESCoP} - Q_{t,DDScat}|}{|Q_{t,DDScat}|}$$

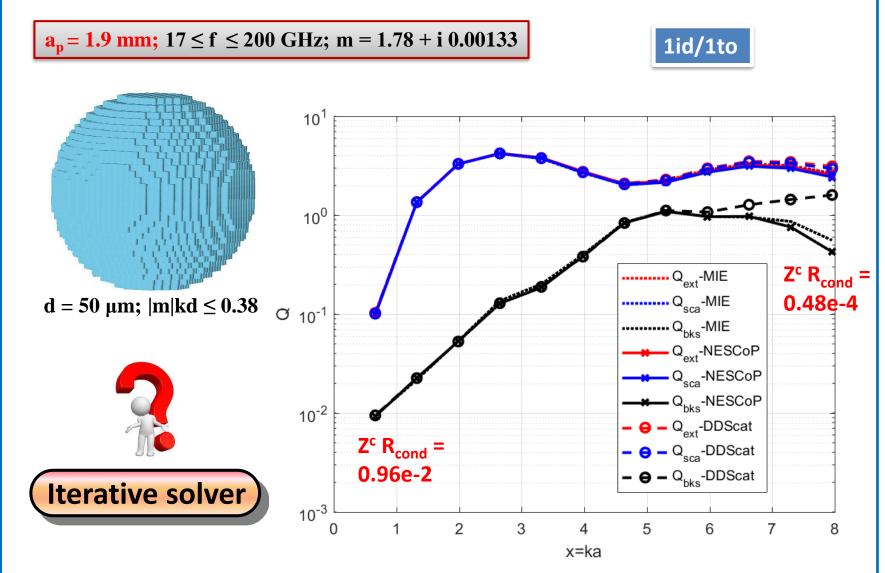










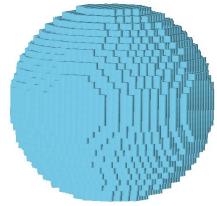






 $a_p = 1.9 \text{ mm}$ ;  $17 \le f \le 200 \text{ GHz}$ ;  $m = 1.78 + i \ 0.00133$ 

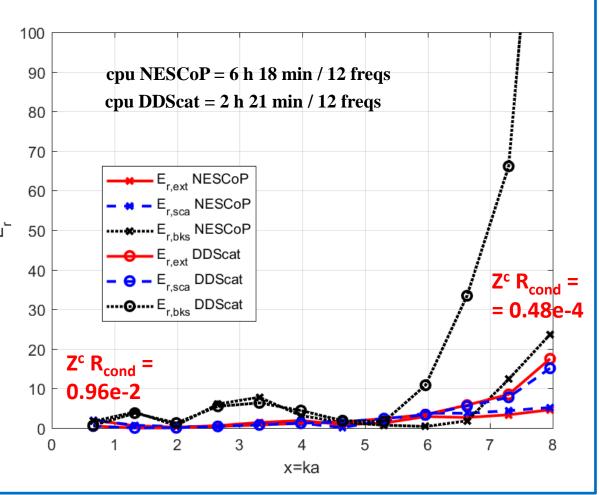
1id/1to



 $d = 50 \mu m$ ;  $|m|kd \le 0.38$ 



**Iterative solver** 







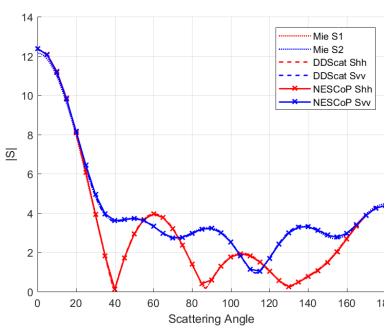
$$a_p = 1.9 \text{ mm}$$
;  $m = 1.78 + i \ 0.00133$ 

$$d = 50 \mu m$$
;  $Nb_c = 229423$ 

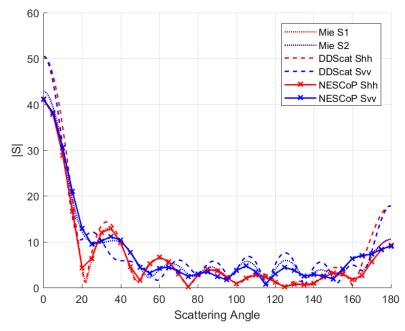
1id/1to

#### f = 100 GHz; |m|kd = 0.18; x = 3.14





>ZBCG2 IT= 31 f.err= 3.726E-05 >ZBCG2 IT= 32 f.err= 4.769E-06 >TIMEIT Timing results for: PBCGS2 >TIMEIT 1555.523 = CPU time (sec)



>ZBCG2 IT= 538 f.err= 1.119E-05 >ZBCG2 IT= 539 f.err= 9.469E-06 >TIMEIT Timing results for: PBCGS2 >TIMEIT 25824. = CPU time (sec)





$$a_{\rm p} = 1.9 \text{ mm}; \text{ m} = 1.78 + i \ 0.00133$$

$$d = 50 \mu m$$
;  $Nb_c = 229423$ 

200

150

100

50

-50

-100

-150

phase(S) (deg)

1id/1to

Mie S1

Mie S2

**DDScat Shh** 

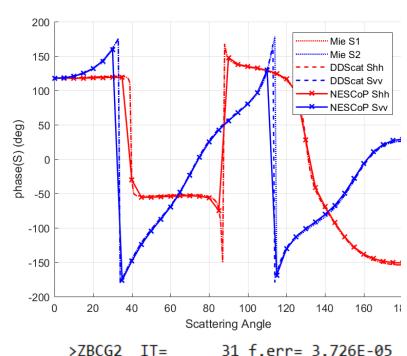
DDScat Svv

NESCoP Shh

NESCoP Svv

#### f = 100 GHz; |m|kd = 0.18; x = 3.14

f = 200 GHz; |m|kd = 0.37; x = 7.96



-200 20 40 60 80 100 120 140 160 180 Scattering Angle >ZBCG2 538 f.err= 1.119E-05 IT= >7BCG2 539 f.err= 9.469E-06 Timing results for: PBCGS2 >TIMEIT >TIMEIT 25824. = CPU time (sec)

>ZBCG2 IT= 31 f.err= 3.726E-05 >ZBCG2 IT= 32 f.err= 4.769E-06

>TIMEIT Timing results for: PBCGS2

>TIMEIT 1555.523 = CPU time (sec)



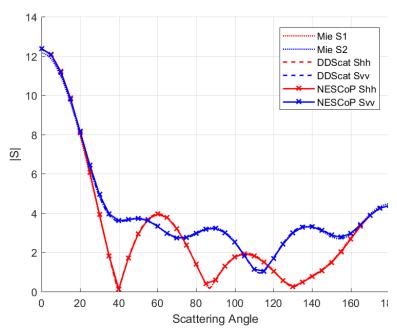


$$a_{\rm p} = 1.9 \text{ mm}; \text{ m} = 1.78 + i \ 0.00133$$

$$d = 50 \mu m$$
;  $Nb_c = 229423$ 

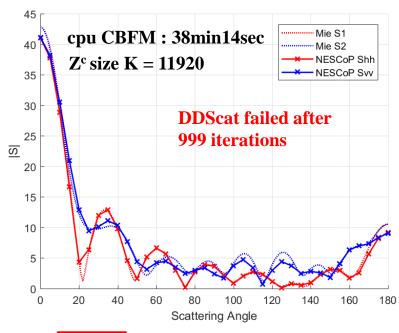
1id/1to

#### f = 100 GHz; |m|kd = 0.18; x = 3.14



>ZBCG2 IT= 31 f.err= 3.726E-05 >ZBCG2 IT= 32 f.err= 4.769E-06 >TIMEIT Timing results for: PBCGS2 >TIMEIT 1555.523 = CPU time (sec)

#### f = 200 GHz; |m|kd = 0.37; x = 7.96



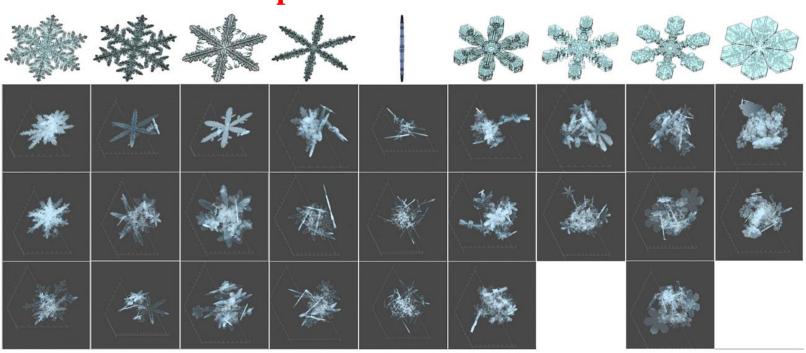
>QMRCCG IT= 998 f.err= 2.436E-01 >QMRCCG IT= 999 f.err= 2.436E-01

real 25m39.069s

### Ice-phase particle modeling : OpenSSP database



### **OpenSSP** database



(top) Pristine crystal types simulated using the snowfake algorithm [adapted from Gravner and Griffeath (2009)] Beneath each type are snapshots of the aggregation simulation that is based upon each crystal type.

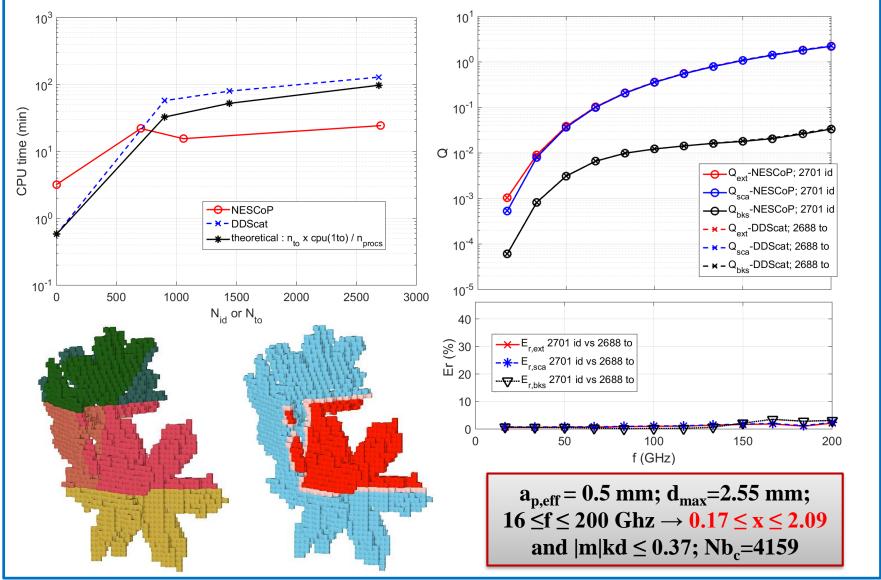
[1] Kuo, K. S., Olson, W. S., Johnson, B. T., Grecu, M., Tian, L., Clune, T. L., ... & Meneghini, R. (2016). The Microwave Radiative Properties of Falling Snow Derived from Nonspherical Ice Particle Models. Part I: An Extensive Database of Simulated Pristine Crystals and Aggregate Particles, and Their Scattering Properties. Journal of Applied Meteorology and Climatology, 55(3), 691-708.

- ➤ 6646 particles : single pristine crystals and aggregate snow particles
- > 50 μm resolution

ftp://gpmweb2.pps.eosdis.nasa.gov/pub/OpenSSP/

a0072



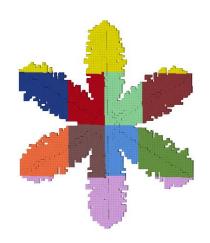




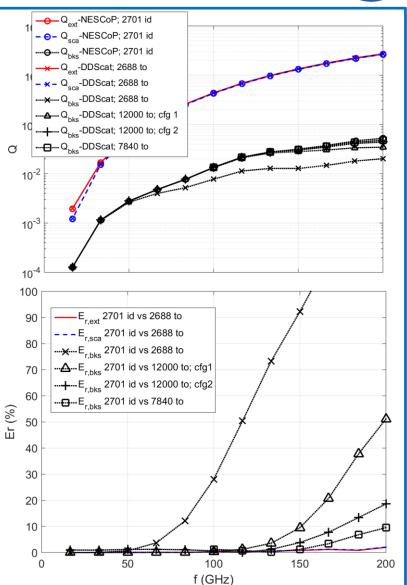


$N_{to}$	$N_{\beta}, N_{\theta}, N_{\Phi}$	$E_{r,ext/scat}$	$E_{r,bks}$	time
2688	16, 12, 14	2.05	159.2	65.37
14520	22, 30, 22	2.32	127.9	274.9
14616	58, 36, 7	2.34	107.9	562.17
10000	10, 50, 20	2.37	63.19	199.78
12000	8, 60, 25	2.36	51.15	213.5
12000	30, 80, 5	2.39	18.6	607.32
5700	60, 95, 1	2.4	13.04	1182
7840	80, 98, 1	2.39	9.52	1974.6

Time (min) and maximum relative difference (%) obtained with DDScat for the ice pristine p08 in comparison to NESCoP with 2701 id, depending on the number of target orientations  $N_{to}$  and on their distribution.

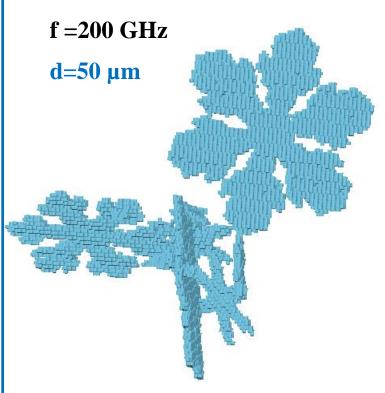


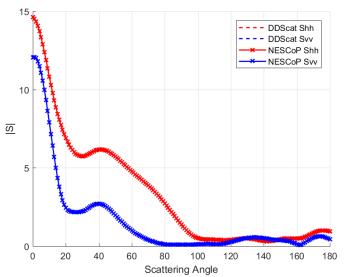
 $a_{p,eff} = 0.58 \text{ mm};$   $d_{max} = 4.30 \text{ mm};$   $0.2 \le x \le 2.49$   $|m|kd \le 0.37;$   $Nb_c = 6738$ 





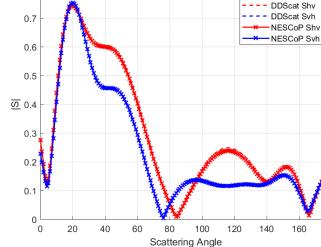








**DDScat** 1 min 18 sec



**NESCoP** 1 min **10** sec

160

 $d_{max}=5.6$  mm; x = 11.72;|m|kd = 0.37;  $D_{\lambda} = 16$  $Nb_c = 11148$  cells

8.0



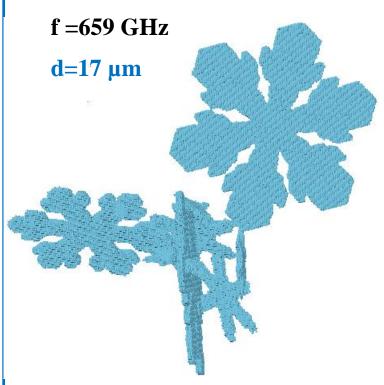
DDScat Shv DDScat Svh

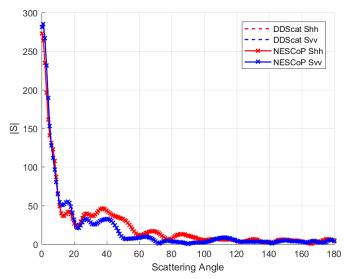
NESCoP Shv

140

160

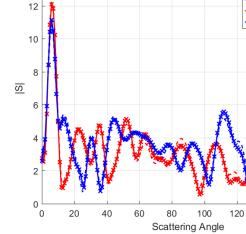








DDScat 16 h



NESCoP 1 h 8 min

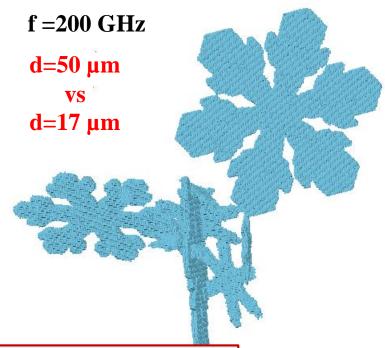
 $|m|kd = 0.41; D_{\lambda} = 15$  $Nb_{c} = 303034 \text{ cells}$ 

 $d_{\text{max}}$ =5.6 mm; x = 38.66;

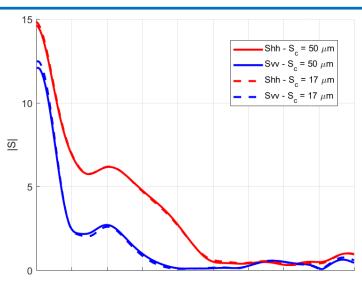


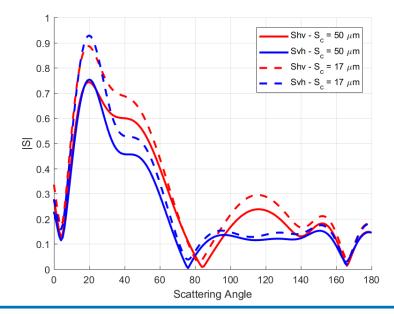


### Impact of d



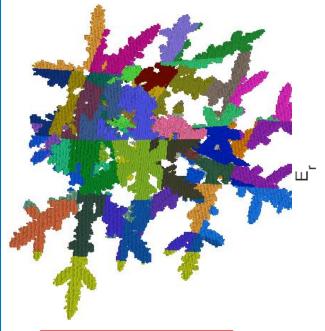
 $d_{max}$ =5.6 mm; x = 11.72; |m|kd = 0.37;  $D_{\lambda} = 16$ vs |m|kd = 0.12;  $D_{\lambda} = 50$ 



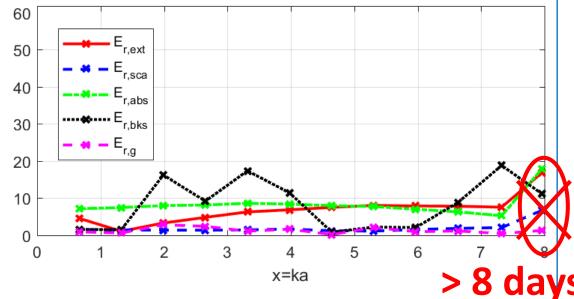








### 180 to $(N_{\theta}=18; N_{\phi}=10) / 1891 id (N_{\theta}=31; N_{\phi}=61)$



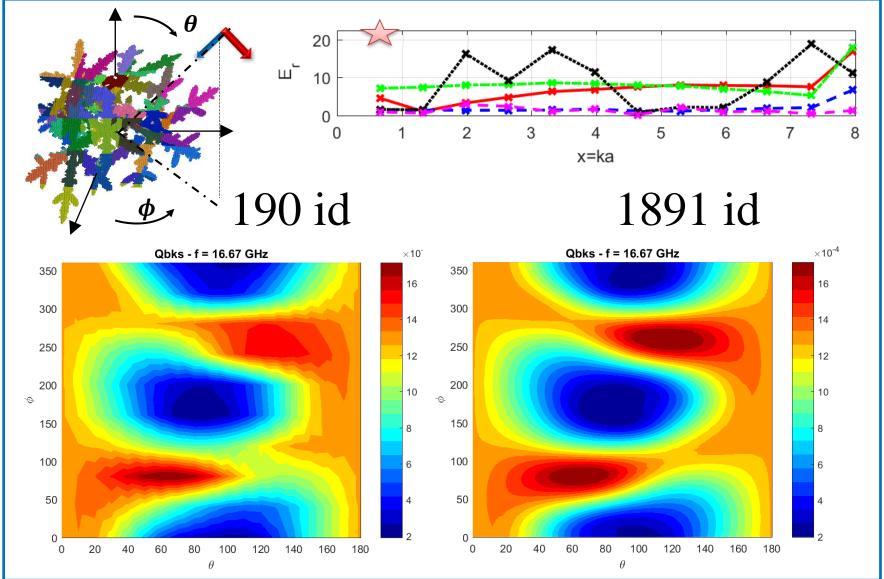
 $a_{eff} = 1.61 \text{ mm};$   $d_{max} = 11.45 \text{ mm};$   $2 \le x \le 24$   $|m|kd \le 0.37$   $Nb_c = 140896 \text{ cells}$ 

### OpenMP; 64 GB of RAM; 16 cpus

DDScat (180 to)	190 id	703 id	1891 id
> 59 days	5 hours	12 hours	23 hours

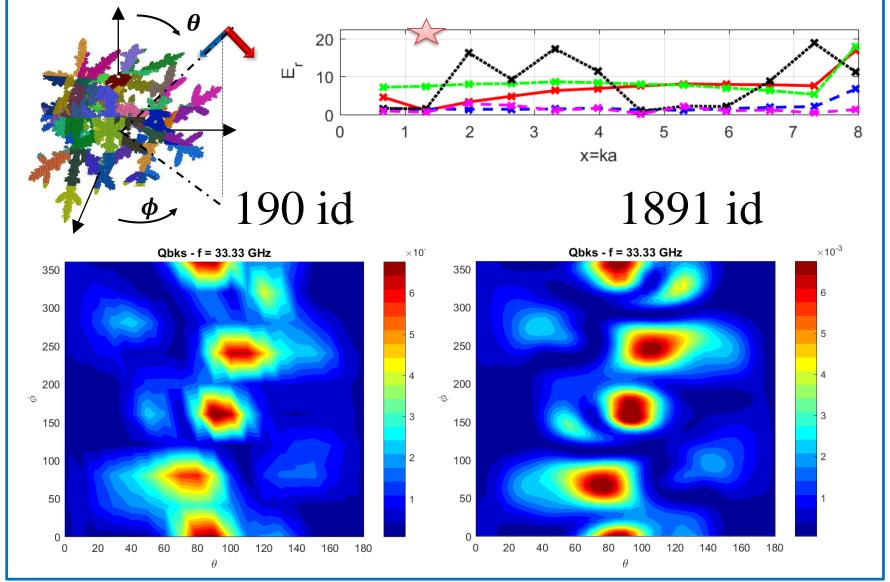






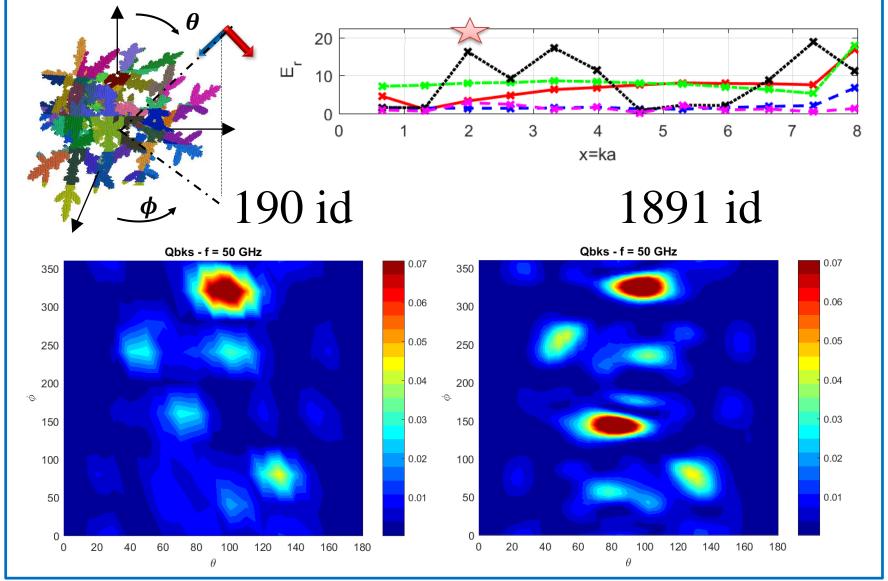






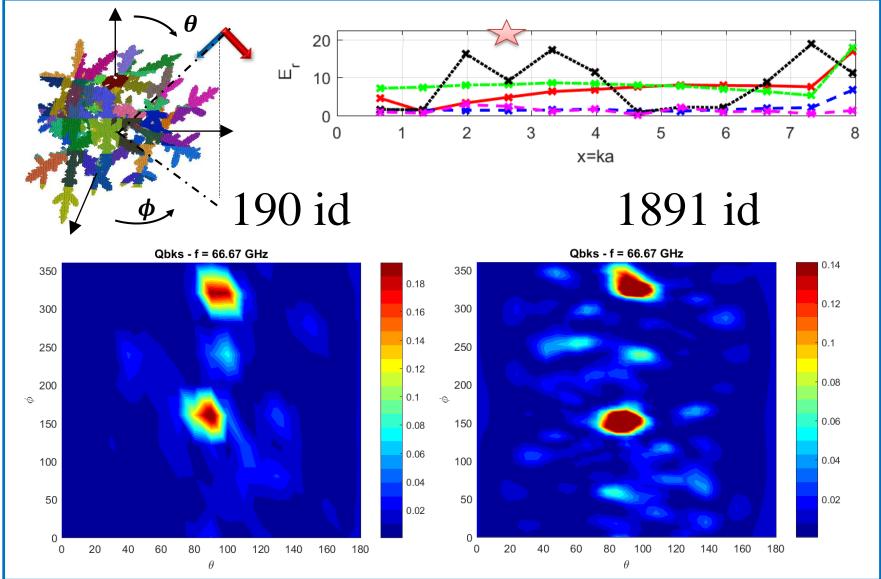






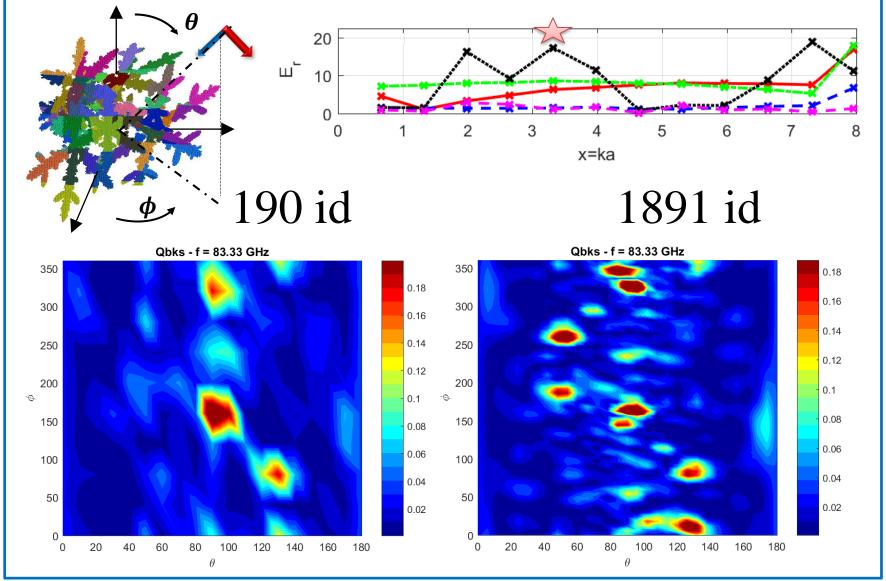






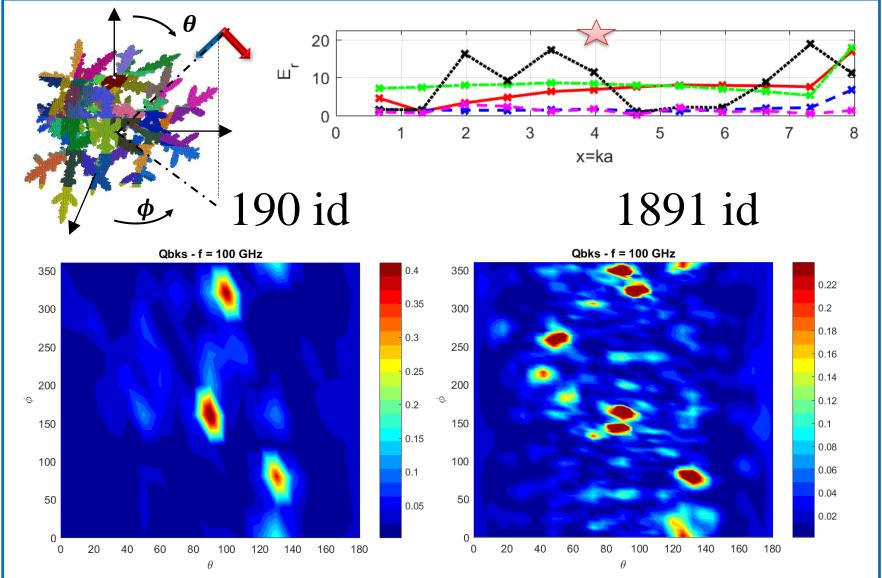






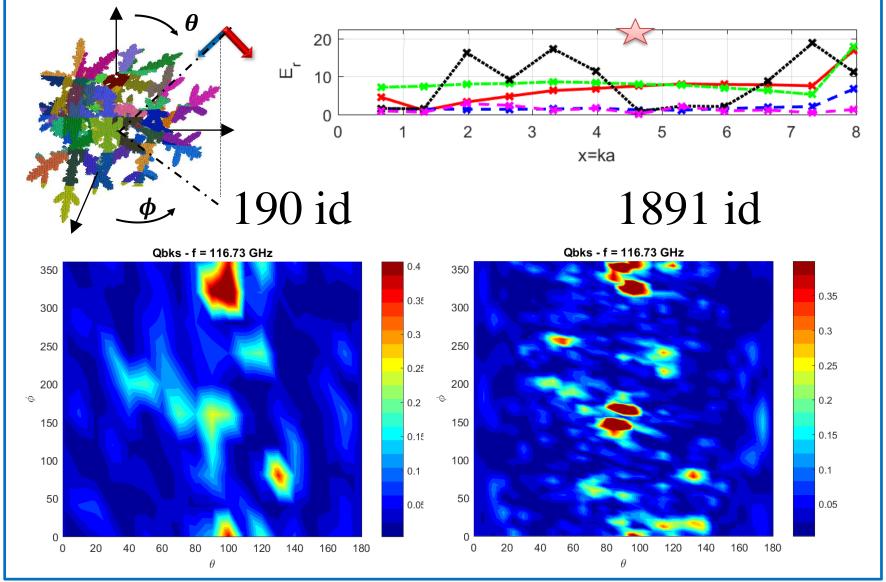






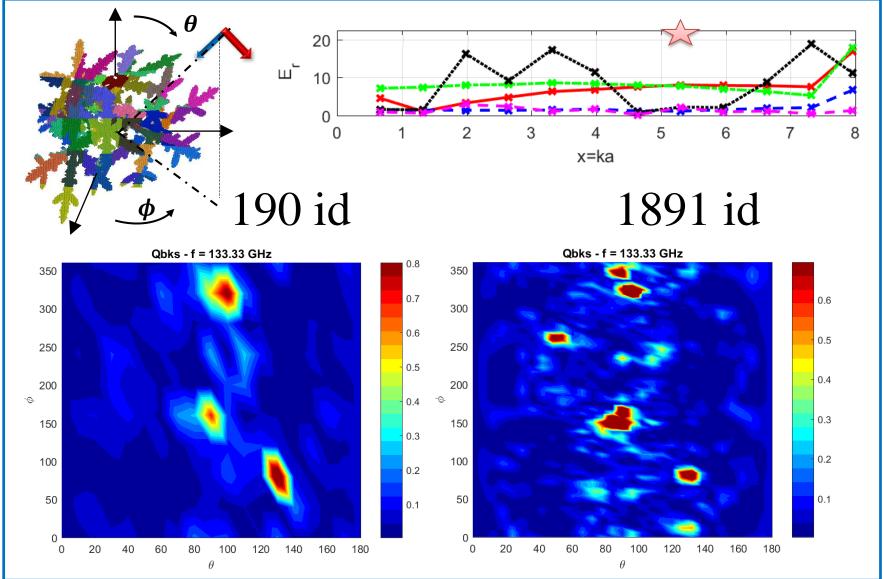






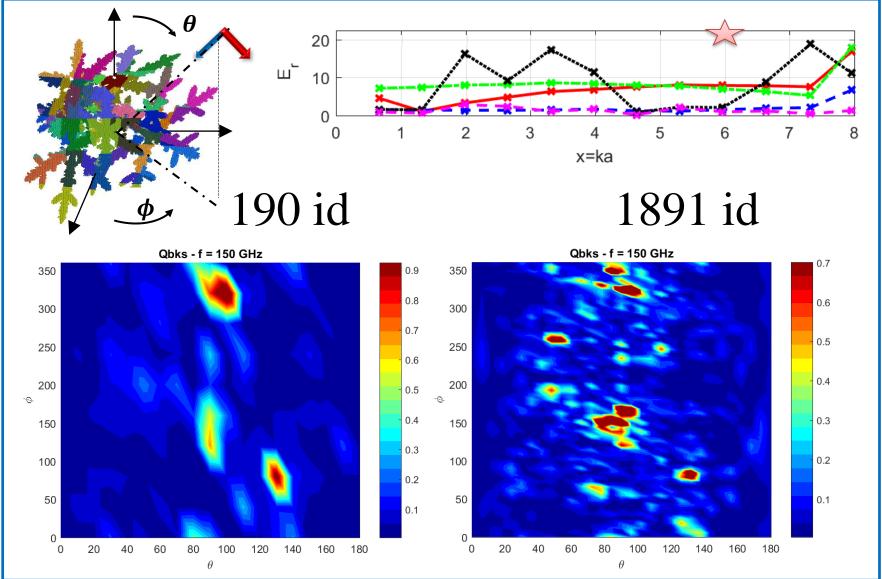






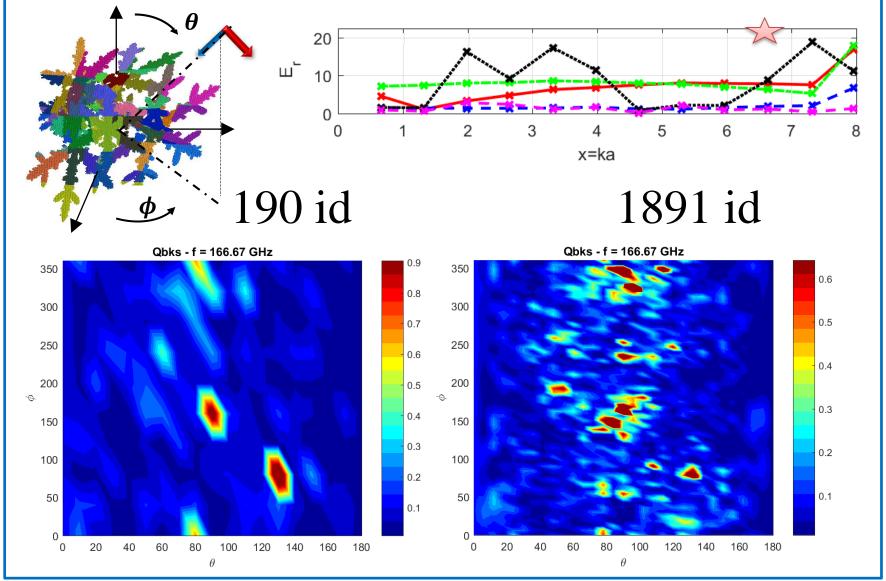






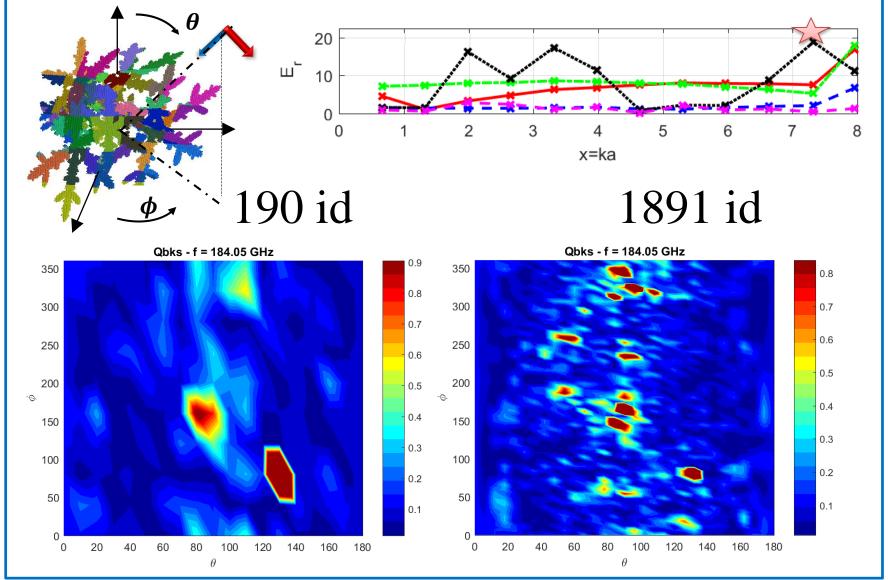






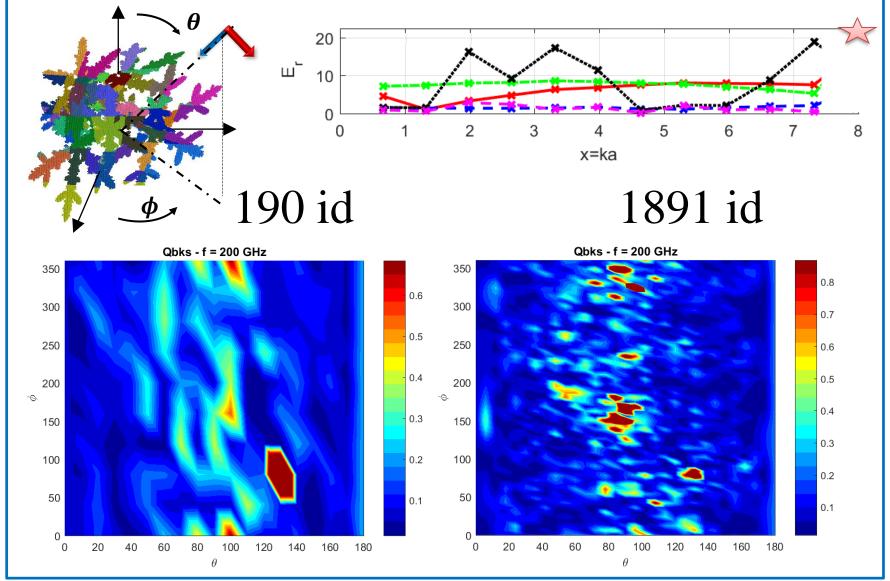












## **Conclusions and Perspectives**



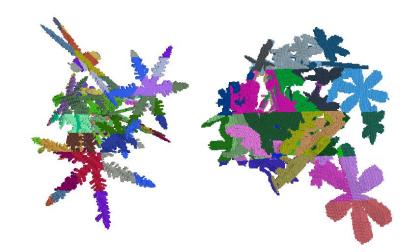


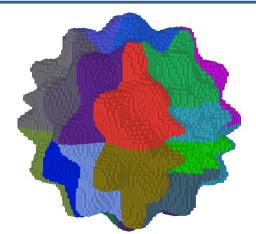


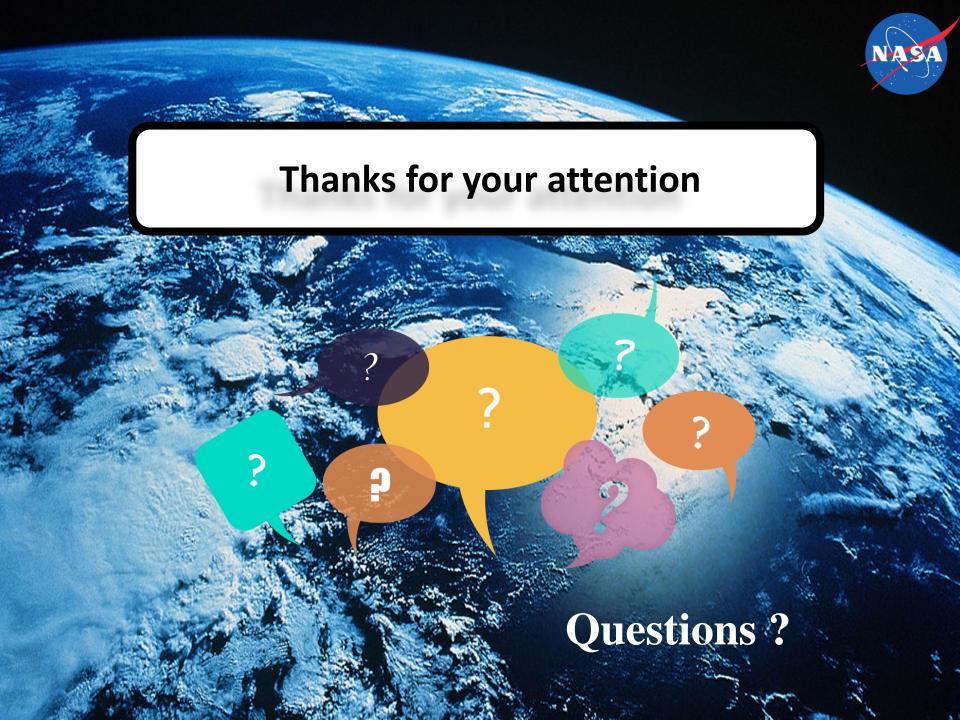


3D full wave model comparable to the DDA in terms of accuracy when providing **higher computational performance** particularly with orientational averaging of the EM scattering.

- ❖ MPI parallelization of the codes
- ❖Exploring different techniques for efficient calculation of the CBFs
- ❖ Adaptation of the domain decomposition and CBFs calculation to 3D Chebyshev/Gaussian Random particles







a0006



